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Al–Th intermetallic compounds. I.

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In the course of an investigation of the system Al–Th we have discovered the existence of six intermetallic compounds, three of which will be described here.

The alloys were prepared by melting pressed mixtures of thorium and aluminum powder in an argon-arc furnace on a water-cooled copper plate. After homogenizing, the specimens were crushed and the powder was sieved until a grain size $< 50\,\mu$ was attained. The powder was then annealed *in vacuo* for $\frac{1}{2}$ hr. at 600–650° C.

Powder-diffraction patterns were obtained by means of a 'Norelco' diffractometer with Cu $K\alpha$ radiation (λ Cu $K\alpha_1 = 1{\cdot}54050$ Å).

I. Al_3Th

This phase was isolated earlier by Leber (1927). Brauer (1938) determined its crystal system to be hexagonal with $a = 6{\cdot}480$ kX., $c = 4{\cdot}601$ kX. $A = 8$. We have measured 54 lines. The results are:

Space group: $P6_3/mmc$ (No. 194);
$a = 6{\cdot}499$, $c = 4{\cdot}626$ Å;
$Z = 2$;
$d_o = 6{\cdot}14$, $d_c = 6{\cdot}14$ g.cm.$^{-3}$;
Th in $2d$: $\pm(\frac{2}{3}, \frac{1}{3}, \frac{1}{4})$,
Al in $6h$: $\pm(x, 2x, \frac{1}{4})$, $\pm(2\bar{x}, \bar{x}, \frac{1}{4})$, $\pm(x, \bar{x}, \frac{1}{4})$ with $x = 0{\cdot}143$;
$\sum_{25} |I_o - I_c| \div \sum_{25} I_o = 7{\cdot}9\,\%$.

Each Th atom is surrounded by 3×2 Al atoms at a distance 3·26 Å, 2×3 Al atoms at 3·15 Å, 2×3 Th atoms at 4·408 Å and 2 Th atoms at 4·627 Å.

Strings of triangular groups of Al atoms run along the c axis. Each Th atom is in 'contact' with 4 Al atoms in each of three strings. Within the strings the Al–Al distances are 2·79 Å and 2·82 Å. The closest distance between Al atoms in different strings is 3·71 Å.

II. Al_2Th

Of this compound we measured 41 lines. Our results are:

Space group: $P6/mmm$ (No. 191);
$a = 4{\cdot}393$, $c = 4{\cdot}164$ Å;
$Z = 1$;
$d_o = 6{\cdot}84$, $d_c = 6{\cdot}85$ g.cm.$^{-3}$;
Th in $1a$: (0, 0, 0),
Al in $2d$: $\pm(\frac{2}{3}, \frac{1}{3}, \frac{1}{2})$;
Structure type: $C32$ (AlB_2);
$\sum_{39} |I_o - I_c| \div \sum_{39} I_o = 13{\cdot}8\,\%$.

The structure does not need to be described. The very short Al–Al distance of 2·54 Å is remarkable, but the structure has been further confirmed by neutron-diffraction analysis (Andresen & Goedkoop, 1955). A comparable short Al–Al distance was found by Nowotny (1942) in Al_4Ce and Al_4La.

The other distances are

Th–Al = 3·28 Å, Th–Th = 4·166 Å and 4·394 Å.

III. Al_2Th_3

This compound appeared to be stable only above 1100° C. The specimen was prepared by heating the alloy, made in the argon-arc furnace, for 2 hr. *in vacuo* at 1200° C. After crushing and sieving, the diffraction diagram was made, without annealing the powder. Our results are:

Space group: $P4/mbm$ (No. 127);
$a = 8{\cdot}13$, $c = 4{\cdot}22$ Å;
$Z = 2$;
$d_o = 8{\cdot}98$, $d_c = 9{\cdot}02$ g.cm.$^{-3}$;
Th in $2a$: (0, 0, 0), $(\frac{1}{2}, \frac{1}{2}, 0)$,
Th in $4h$: $\pm(x, \frac{1}{2}+x, \frac{1}{2})$, $\pm(\frac{1}{2}+x, \bar{x}, \frac{1}{2})$ with $x = 0{\cdot}674$,
Al in $4g$: $\pm(y, \frac{1}{2}+y, 0)$, $\pm(\frac{1}{2}+y, \bar{y}, 0)$ with $y = 0{\cdot}116$;
$\sum_{36} |I_o - I_c| \div \sum_{36} I_o = 20{\cdot}3\,\%$.

The structure of Al_2Th_3 can be imagined as being built up of a network of pseudo-cubic 'Th' and pseudo-hexagonal 'Al_2Th'. Fig. 1 demonstrates this peculiar

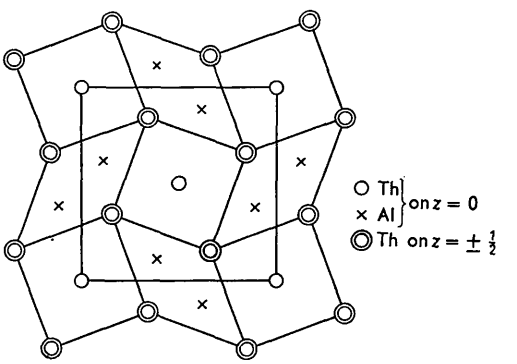

Fig. 1. Projection of cell of Al_2Th_3 on basal plane.

feature. The pseudo-cubic parts have $c/a = 0{\cdot}99$. The 'Al_2Th' parts are not exactly hexagonal (they would be so for a Th parameter $x = 0{\cdot}683$).

A Th atom at $z = 0$ has 8 Th neighbours at 3·67 Å, 2 Th at 4·22 Å and 4 Al neighbours at 3·26 Å. A Th atom at $z = \frac{1}{2}$ has 1 Th neighbour at 4·00 Å, 2 Th at 4·22 Å and 4 Th at 4·25 Å. Moreover, it has 6 Al neighbours at 3·20 Å.

Data, containing spacings, indices and intensities of these three compounds, have been sent to the Committee of the A.S.T.M. card index for X-ray diffraction data.

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